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Lattice effects in YVO_3 single crystal

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Abstract

In this paper we report on the lattice effects in the Mott insulator yttrium orthovanadate (YVO_3). Linear thermal expansion and magnetostriction experiments have been performed on a single crystal, in the temperature range from 5 K to room temperature. The YVO_3 orders antiferromagnetically at $T_N = 116$ K and orbital ordering was reported to appear below $T_{OO} = 196$ K. A first-order structural phase transition takes place at $T_S = 77$ K, accompanied by changes in the antiferromagnetic type of ordering as well as in the orbital-ordering type. Our results reveal that the thermal expansion measurement technique is a very powerful tool in order to clearly detect the existence of the above-mentioned transitions. The magnetostriction results point to the stability of the low-temperature-magnetic ground state under such high applied magnetic field.

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Keywords: Thermal expansion; Mott localization; Phase transitions—structural; Magnetostriction

Yttrium orthovanadate (YVO_3) presents a distorted perovskite structure. It is a Mott insulator where the 3d V^{3+} magnetic moments order antiferromagnetically (AF) below $T_N = 116$ K. At temperatures higher than $T_S = 77$ K the spin order (SO) is C-type AF (ferromagnetic coupling along *c*-axis and AF within the *ab* planes), whereas below T_S a change to a G-type AF structure (AF coupling in all directions) takes place through a first-order structural phase transition accompanied by a change in the unit cell volume [1]. A Jahn–Teller-ordered state at low temperature evidences the existence of orbital ordering (OO) which symmetry changes at T_S from G-type (all d_{xy} orbitals occupied and alternatively occupied d_{yz} and d_{zx} ones) to C-type (alternative occupation within *ab* planes and the same along *c*-axis) while cooling. In spite of the lack of SO above T_N the OO remains up to $T_{OO} = 196$ K, where a next structural phase transition takes place [2,3]. The changes of the OO structure of the YVO_3 have been proposed as the origin of the observed multiple temperature-induced magnetisation reversal processes [4].

Similar OO transitions as well as the magnetic transitions are the common features of whole family of the RVO_3 orthovanadates (R being a rare-earth ion), whereas the first-order structural phase transition has been observed only in the compounds where R = Lu, Yb, Er, Dy [5]. On the other hand, previous magnetisation results obtained in oriented powder-samples of the $Y_{1-x}Ca_xVO_3$ series [6] suggest also the existence of metamagnetic transitions at high magnetic fields.

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In order to have a deeper insight into the lattice and volume changes associated to the mentioned structural, magnetic- and orbital-ordering transitions we have performed linear thermal expansion measurements (LTE). The relative length change due to thermal expansion has been measured using the strain gauge technique: the relative resistance change of a gauge fixed on the sample (in this case parallel to each of the three crystallographic axes), is proportional to the relative length change $\Delta l/l$. The LTE measurements have been performed in the temperature range between 300 K and liquid helium temperature. The experiments were performed cooling and subsequently heating the sample, in both cases at a temperature rate of 0.5 K/min. The data were taken every 0.1 K. Details about the single crystal preparation can be found in Ref. [3].

The LTE along the three crystallographic axes measured when the temperature is increased, is shown in Fig. 1(a), while Fig. 1(b) presents the temperature dependence of the LTE coefficient α, which is defined as the first derivative of the LTE. The calculated volume thermal expansion and volume expansion coefficient are displayed in Fig. 1(c). The measurements show that the LTE has strong anisotropic character. Nevertheless, the measurements along the three crystallographic directions display some common features. When increasing the temperature an abrupt anomaly is observed at $T_S = 77$ K, which corresponds to a simultaneous contraction along the a- and c-axis ($\Delta l/l \approx 0.15$ and 0.20%, respectively) together with an expansion along the b direction ($\Delta l/l \approx 0.5$). These values are in good agreement with the lattice parameter distortion values derived from neutron scattering experiments [1]. The comparison of the LTE measurements, performed while cooling and heating the sample, reveals the existence of hysteresis in the structural transition, and therefore confirms the first-order character of this transition. This is clearly seen in the inset of Fig. 1(a), where the LTE along the c-axis in the vicinity of T_S is displayed. The values of the LTE decreasing and increasing the temperature are the same, which confirms the reversibility of the first-order transition. These features have been observed along the three crystallographic axes (though not displayed here for the sake of clarity). The abrupt change in the crystal dimensions could be the reason of the contact loss between sample and sample-holder observed in the specific heat measurements at T_S [3]. Increasing the temperature above T_S, the progressive expansion of the a and c lattice parameters and the simultaneous decrease of the b-axis take place. Very weak anomalies (slope decrease) are detected in the LTE at the magnetic order transition temperature $T_N \approx 116$ K. Nevertheless, the magnetic order transition is nicely revealed in the $\alpha(T)$ dependencies, shown in Fig. 1(b), as a decrease of absolute value of LTE coefficient by $0.1 \times 10^{-5}\,\mathrm{K}^{-1} \leqslant \alpha \leqslant 0.5 \times 10^{-5}\,\mathrm{K}^{-1}$.

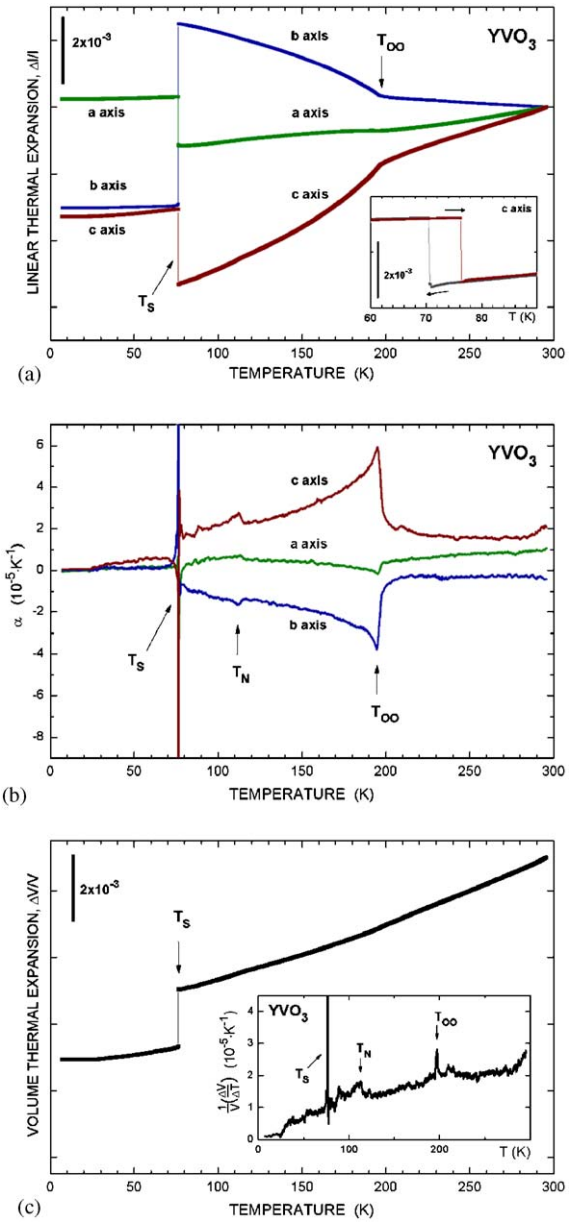

Fig. 1. (a) LTE along the three crystallographic axes. The results have been taken while heating. Inset: LTE along the c-axis in the vicinity of T_S, while cooling and heating the sample. (b) LTE coefficient, α, and (c) volume thermal expansion and its coefficient (inset) of an YVO_3 single crystal. The temperatures of the orbital order (T_{OO}), magnetic order (T_N), and the first-order structural (T_S) transitions are marked by arrows. The absolute values of α as well as volume expansion coefficient at T_S are much higher than the graph limits.

Moreover, a drastic slope change is observed at $T_{OO} = 196$ K, which coincides with the appearance of a sharp peak in the specific heat measurements, which was associated with the OO transition [3]. This anomaly

is specially marked in the LTE measured along the b and c axes. Nevertheless, the $\alpha(T)$ dependencies show that all three crystal directions are involved in creation of the G-type orbital order.

The corresponding relative volume change with respect to the initial sample volume (see Fig. 1(c)) is $\Delta V/V \approx 0.20$. The thermal dependence of the volume shows the drastic change at T_S already seen in the LTE. Nevertheless, the absence of significant volume changes at highest temperatures indicates that the transition taking place at T_{OO} is really an effect related to the ordering of the electronic orbitals.

In order to elucidate the stability of the low-temperature magnetic and orbital ordered state of YVO_3 under applied magnetic field, we carried out high-field magnetostriction measurements. The experiments were performed in the long-pulsed magnetic field facility (30 T maximum available magnetic field) at the University of Zaragoza-CSIC. Magnetostriction isotherms were measured at several temperatures ($T = 300$, 250, 220, 200, 150, 120, 100, 80, 60, 40, 20, 10 and 5 K). The deformation was measured along the a, b, and c crystallographic axes when the crystal was subsequently oriented parallel and perpendicular to the applied magnetic field. For all the crystal orientations the magnetostriction at the maximum applied field is zero ($\pm 10 \times 10^{-6}$) at temperatures above 80 K. Decreasing the temperature, the magnetostriction increases gradually up to $\approx 100 \times 10^{-6}$, but this variation corresponds to the magnetoresistance of the strain gauge itself. Therefore, we can consider that the magnetostriction is almost negligible in the whole temperature range and no significant features or changes that could be associated to the structural, orbital or magnetic order transitions have been observed. Therefore, these results confirm the stability of the low-temperature orbital and magnetic state under an applied magnetic field.

In summary, we measured LTE and magnetostriction in a YVO_3 single crystal in the temperature range from 5 to 300 K. Magnetostriction measurements did not reveal any magnetic-induced phenomena. LTE measurements showed an anisotropic character and gave direct evidence of the creation of the orbital ordered state below $T_{OO} = 196$ K and of the abrupt change of structure at $T_S = 77$ K. The magnetic (spin) ordering was also recognised in the temperature dependence of the LTE coefficient α.

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References

[1] H. Kawano, et al., J. Phys. Soc. Jpn 63 (1994) 2857.
[2] G.R. Blake, et al., Phys. Rev. Lett. 87 (2001) 245501.
[3] G.R. Blake, et al., Phys. Rev. B 65 (2002) 174112.
[4] Y. Ren, et al., Nature 396 (1998) 441.
[5] S. Miyasaka, et al., Phys. Rev. B 68 (2003) 100406(R).
[6] H. Nakotte, et al., Int. J. Mod. Phys. B 16 (2002) 3041.